

عنوان مقاله:

The study of drug resistance properties of ABCG₂ (ATP-binding cassette G₂) in contact with thymoquinone, gallic acid, and hesperetin antioxidants

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خلاصه مقاله:

Introduction: ATP-binding cassette (ABC) transporters are a group of intra membrane proteins that play key roles in the transmission and exchange of vital compounds on both sides of the membrane. These proteins can specially transport anti-cancer drugs out of cancer cells. ABCG₂ is a member of this family that is extremely expressed in many cancers. This study, aims to evaluate the binding affinity of three antioxidants thymoquinone (TQ), gallic acid (GA), and hesperetin (HP) to ABCG₂ compared with an anti-cancer drug, mitoxantrone (Mit), to export cells. Methods: The PDB file of ABCG₂ was obtained from the protein data bank server (<http://www.rcsb.org>) with ID: 5NJ3. After ۲۰۰ stages of molecular docking running on ABCG₂ protein in AutoDock v.۴.۲ software, the amino acids involved in the binding site of each compound were identified using the LigPlot+ software. Results: HP had the lowest (-۶.۳۶ kcal/mol) and GA had the highest (-۳.۹۳ kcal/mol) binding energy in comparison with Mit (-۰.۰۶ kcal/mol) for binding to ABCG₂. Effective concentration required to perform the reaction between ABCG₂ was higher in GA (۱.۳۱ mM) than TQ (۴۲.۶۹ μM) and HP (۲۱.۷۴ μM). GA, HP, and TQ formed ۱۷, ۱۸, and ۲۲ hydrogen and hydrophobic bonds at the binding site of ABCG₂. Conclusion: It seems that GA has the lowest affinity to make contact with ABCG₂ binding site. So, GA tends to remain in the cell but TQ and HP tend to leave the cell easily via ABCG₂ transporter.

کلمات کلیدی:

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